



Co-Optimization of  
Fuels & Engines

Project ID: FT057

## Co-Optimization of Fuels and Engines (Co-Optima): Emissions, Emission Control, and Sprays

Todd J. Toops  
Lyle Pickett, Chris Powell,  
Bob McCormick, Matt Ratcliff,  
John Storey, Melanie DeBusk, Josh Pihl,  
William Brookshear, Sreshtha Majumdar

June 8, 2017



## FY17 Vehicle Technologies Office Annual Merit Review

better fuels | better vehicles | sooner



Energy Efficiency &  
Renewable Energy

Co-Optima DOE VTO Management Team:  
Kevin Stork, Mike Weismiller, Leo Breton, & Gurpreet Singh

*This presentation does not contain any proprietary, confidential, or otherwise restricted information.*



## Timeline

- Project start date: 10/1/2015
- Project end date:\* 9/30/2018
- Percent complete: 56%

## Budget

Advanced Engine Development	FY16 (\$K)	FY17 (\$K)	FY18 (\$K)
<b>ORNL (E.1.3.1):</b> Fuel Impacts on Emissions Control Performance & Durability	341	175	350
<b>ORNL (E.1.3.2):</b> Fuel Impact on GDI PM Formation and Gaseous Emissions During Cold Start	183	188	188
<b>ORNL (E.1.3.3):</b> Fuel Contribution to PM From Kinetically-Controlled Combustion	183	188	188
<b>NREL (E.1.3.4):</b> Fuel Effects on Emissions and Aftertreatment	244	250	250
<b>ANL (E.1.4.1):</b> Studies of Sprays and Mixture Formation	200	200	200
<b>SNL (E.1.4.2):</b> Complete Installation of High-Throughput Spray Facility	1150	1050	212

## Barriers

- **Complexity:** Introduction of new fuels and vehicles involves large number of stake holders with competing value propositions
- **Timing:** schedule for completing R&D and achieving market impact is extremely ambitious

## Partners

- Partners include a total of:
  - 9 national laboratories
  - 13 universities
  - External advisory board
  - Stakeholders

\*Start and end dates refer to three-year life cycle of DOE lab-call projects, Co-Optima is expected to extend past the end of FY18



**Fuels can have a pronounced impact on spray structure, mixture formation, emissions, and emissions control systems for all SI and ACI engine technologies. Projects addressing these areas (FY17 budget):**

- **SNL: High-throughput spray chamber (\$1150K)**
  - Lyle Pickett
- **ANL: X-ray imaging of GDI sprays with alcohol blends (\$200K)**
  - Christopher Powell
- **NREL: Particulate Matter Index (PMI) refinement (\$250K)**
  - Bob McCormick and Matt Ratcliff
- **ORNL: PM formation and oxidation fundamentals (\$376K)**
  - Fuel Impact on GDI PM Formation & Gaseous Emissions During Cold Start
  - Fuel Contribution to PM From Kinetically-Controlled Combustion
  - John Storey and Melanie DeBusk
- **ORNL: Fuel Impacts on Emissions Control Performance & Durability (\$175K)**
  - Todd Toops and Josh Pihl

# Milestones



Milestone	Date
<b>SNL:</b> Design and place contracts for high-throughput chamber components <b>{COMPLETE}</b>	9/30/2016
<b>NREL:</b> Complete GDI (SCE) PM emissions test matrix with objective of improving predictions of PMI <b>{COMPLETE}</b>	9/30/2016
<b>ORNL:</b> Evaluate dual SCR system with ethanol-based fuels to determine parameters that enable the emissions targets <b>{COMPLETE}</b>	9/30/2016
<b>ORNL:</b> Measure catalytic light-off behavior of at least five SI-HPF candidates (encompassing five different functional groups) over a three-way catalyst. <b>{DELAYED due budget reduction, \$350k → \$175k}</b>	3/31/2017 ↓ 9/30/2017
<b>SNL:</b> Install completed lower pressure vessel with high-power (60 kW) heater controls	9/30/2017

# Spray Projects



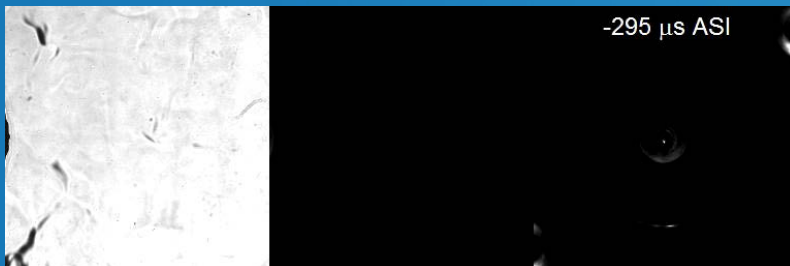
## Project Summary #1

**Sandia National Laboratories**

**High-throughput spray chamber  
(\$1050K)**

**Lyle Pickett (PI)**

Liquid and vapor spray measurements  
of gasoline multi-hole injector



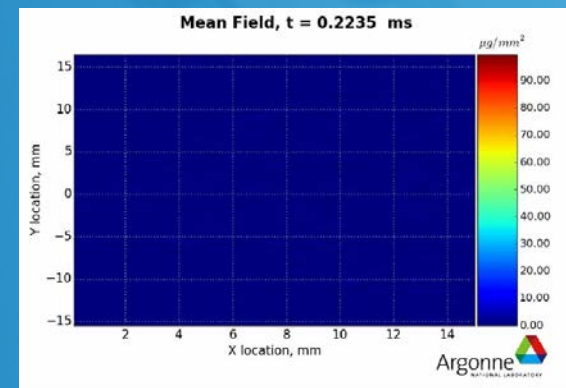
## Project Summary #2

**Argonne National Laboratory**

**X-ray Studies of Sprays and  
Mixture Formation (\$200K)**

**Christopher Powell (PI)**

Daniel Duke, Alan Kastengren,  
Katarzyna Matusik

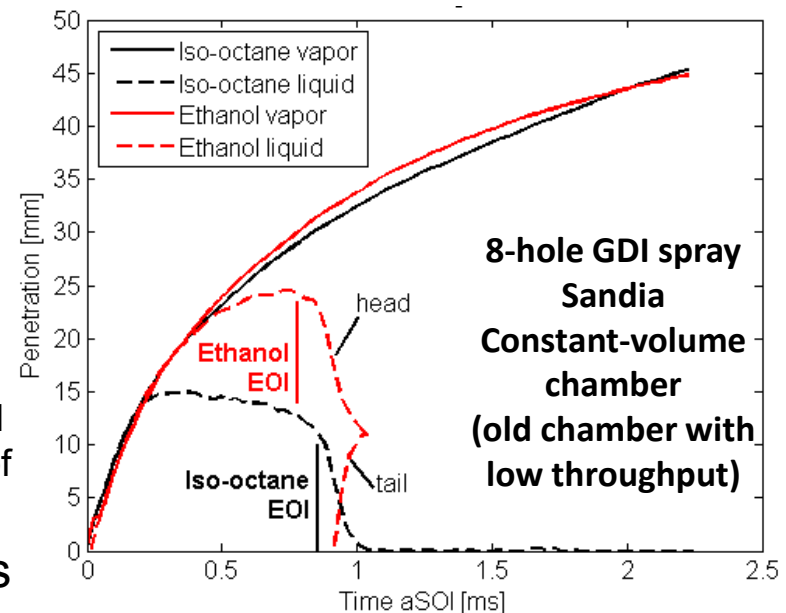






## Objectives and Relevance

- Improve understanding of how fuel properties impact mixture formation
  - Fuel distribution affects ignition, burn-rate, COV, particulate matter, temperature field, knock sites in an engine
- Test the Central Fuels Hypothesis:
  - quantify ways that the physical properties of the fuel affect the fuel distribution and the initial conditions of combustion
- Deliver data for validation of spray simulations



## Approach

- Coordinate spray research efforts at SNL and ANL using the same injector hardware and operating conditions
- **SNL:** Develop and implement a continuous flow spray chamber that reproduces engine T & P and enables a 300X data throughput improvement
  - Large-volume, uniform-temperature (unlike engines or IQT-like chambers)
- **ANL:** Using X-ray technique at the Advanced Photon Source (APS) perform detailed measurements of GDI-based fuel injection sprays



# Approach/Accomplishments

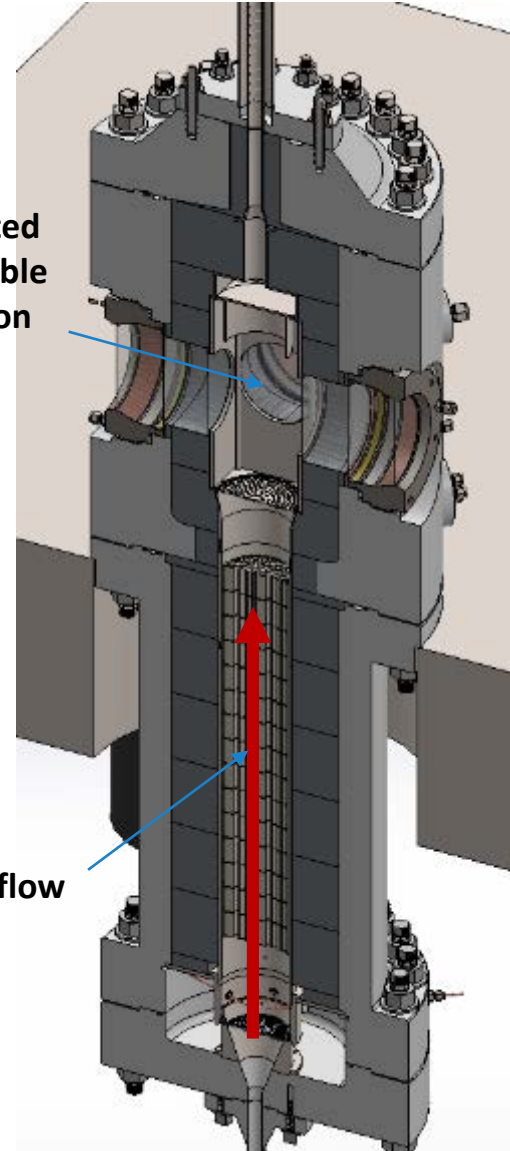
## Status of chamber installation:

- Facility installations in progress:
  - Compressed air and nitrogen to 150 bar
  - Vacuum operation to mimic flash boiling conditions
  - Water cooling system for vessel and exhaust
- Operator room construction:
  - Safety barricade to guard against window failure
  - Heater PID control with intrinsically safe feedback for air flow and cooling flow
- Optical access:
  - Support table with cutouts for chamber anchored to floor for seismic restraint
- Fuel system:
  - Small-volume (50 mL) syringe pump up to 2000 bar for work with small test samples

## Spray Chamber

Thermally isolated  
Optically accessible  
spray test section

Heated air flow  
37 kW  
1100 K





# Approach/Accomplishments

## Status of chamber installation:

- Facility installations in progress:
  - Compressed air and nitrogen to 150 bar
  - Vacuum operation to mimic flash boiling conditions

- Water cooled
- Operator safety:
  - Safety barriers
  - Heater Power feedback

- Optical access:
  - Support structure – expected to contribute to particulate formation and knock.
  - anchored to floor for seismic restraint
- Fuel system:
  - Small-volume (50 mL) syringe pump up to 2000 bar for work with small test samples

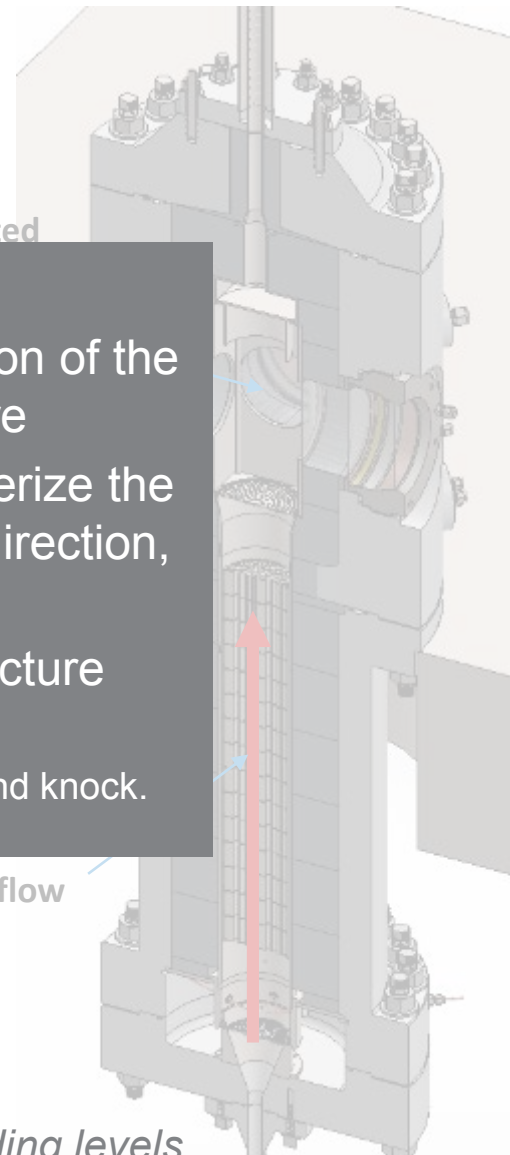
## Future Work/directions

- Characterize the gas temperature distribution of the spray chamber and fuel injector temperature
- For the leading-candidate SI-fuels, characterize the vapor envelope, liquid penetration, plume direction, and droplet size
- Characterize the end-of-injection liquid structure and film formation for all SI-intended fuels

## Spray Chamber

Thermally isolated

Heated air flow  
37 kW  
1100 K



*Any proposed future work is subject to change based on funding levels*



# New High Pressure Fuel System for **Flammable** Fuels



## Progress

- Previous x-ray measurements were limited to combustible, not flammable fuels
  - e.g. diesel, gasoline calibration fluids
- New high pressure fuel system has been procured
  - Suitable for a broad range of fuels at pressure up to 350 bar
- Controls and safety features are currently being implemented

## Deliverables

- Spray breakup will be linked with the physical properties of the fuel
- Fuel impact on mixture formation will be quantified
- Dataset linking fuel properties to mixture formation will be delivered to the modeling community, allowing development and validation of improved spray, combustion, and engine models



New High Pressure Fuel System for **Flammable** Fuels

Project Schedule and Future Plans		
Date	Objective	Status
December 2016	Select a priority list of fuel blend candidates for testing	Complete
March 2017	Complete measurements of the baseline fuel under flash-boiling and non-flashing conditions	Postponed to Q3
June 2017	Complete spray measurements of the selected fuel blends, mapping the fuel/air mixing and its dependence on fuel properties.	On Track
September 2017	Report results	On Track
FY2018	Spray measurements of iso-octane blends with iso-butanol will be tested, studying the triggers of spray collapse	On Track

development and validation of improved spray, combustion, and engine models

*Any proposed future work is subject to change based on funding levels*

# Project Summary #3

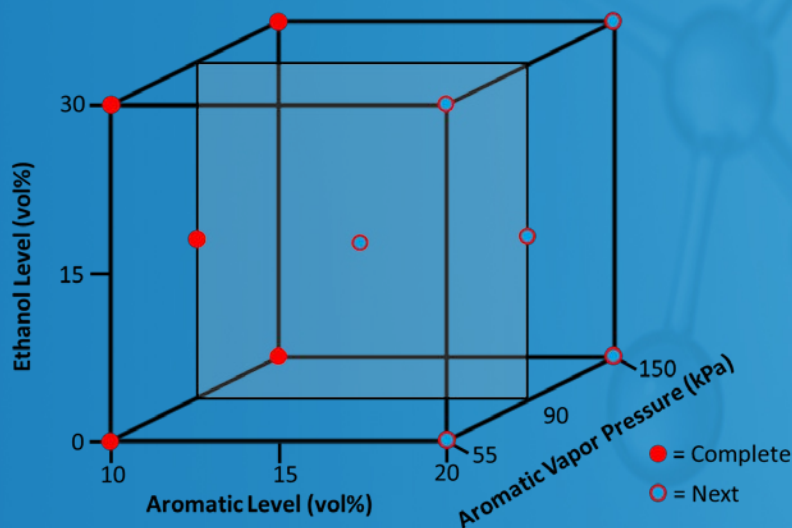


## National Renewable Energy Laboratory

### Fuel Effects on Emissions and Aftertreatment (\$250K)

Bob McCormick and Matt Ratcliff (co-PIs)

Jonathan Burton





# Fine Particle Emissions: Particulate Matter Index (PMI)

## Relevance

- PMI was developed for predominantly hydrocarbon fuels
- Provides a fuel ranking for PM emissions in a given vehicle
- High PMI fuels may require gasoline particle filter
- GPF has a fuel economy impact – backpressure and regeneration
- Honda reported global average PMI to be about 1.6
- The merit function score penalizes engine efficiency by 0.7% if PMI is greater than 1.6
- Increasing penalty if PMI is higher

**Based on detailed hydrocarbon analysis of the base fuel and the quantity of added oxygenate**

$$PMI = \sum_{i=1}^n \left[ \frac{(DBE_i + 1)}{VP(443K)} \times Wt_i \right]$$

Tendency to form soot

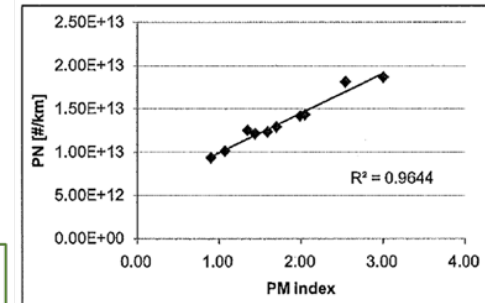
Driver to evaporate and mix with air

Where-

$$DBE = (2C + 2 - H)/2$$

$Wt_i$  = Weight fraction of compound

$VP$  = Vapor pressure at 443K (170°C)



GDI engine equipped cars, FTP-75 bag 1

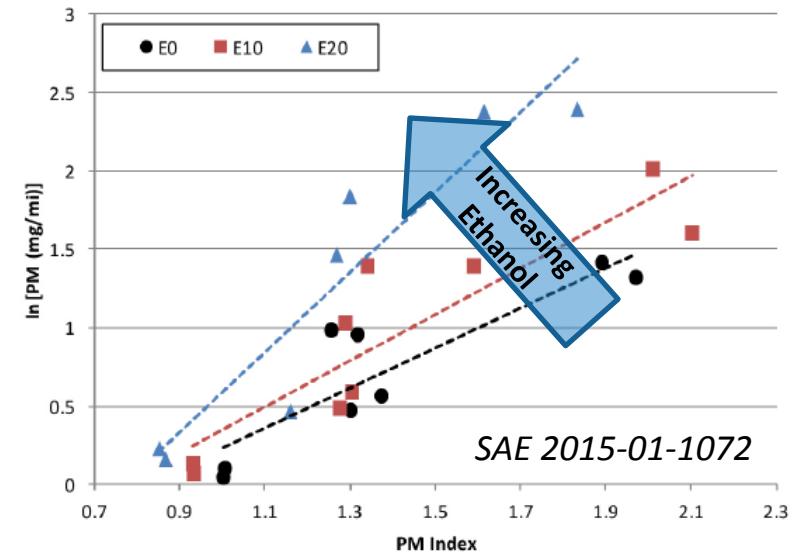
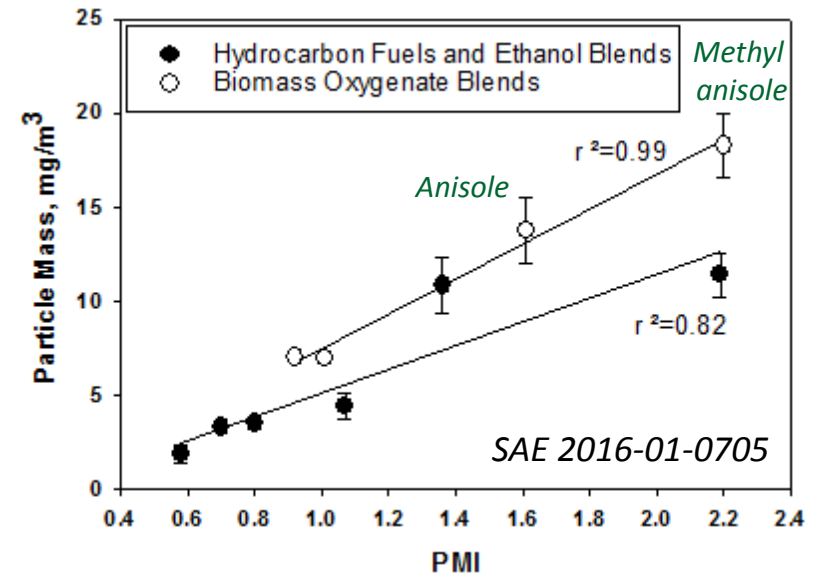
Aikawa, K., Sakurai, T., Jetter, J. J.  
SAE 2010-01-2115

$$\begin{aligned} Merit = & \frac{(RON_{mix} - 91)}{1.6} - K \frac{(S_{mix} - 8)}{1.6} \\ & + \frac{0.085[ON / kJ / kg_{mix}] \cdot ((HoV_{fuel} / (AFR_{stoich} + 1)) - (415[kJ / kg_{fuel}] / (14.3[-] + 1)))}{1.6} \\ & + \frac{((HoV_{fuel} / (AFR_{stoich} + 1)) - (415[kJ / kg_{fuel}] / (14.3[-] + 1)))}{15.38} \\ & + \frac{(S_{Lmix} - 46[cm / s])}{5.4} \\ & - H(PMI - 1.6)[0.7 + 0.5(PMI - 1.4)] \\ & + 0.008^{\circ}C^{-1}(T_{c,90,conv} - T_{c,90,mix}) \end{aligned}$$



# Does PMI Breakdown for Oxygenates?

- Studies of soot formation tendency and soot precursor formation suggest that it will
  - Anisole forms cyclopentadienyl radical which couples to naphthalene (*J. Phys. Chem. A* 2010, 114, 9043–9056)
  - Secondary alcohol dehydration to alkene (*Environ Sci Technol*, 2011, 45 (6), pp 2498–2503)
- High heat of vaporization (from ethanol) may lower effective vapor pressure of high boiling aromatics, increasing PM emissions

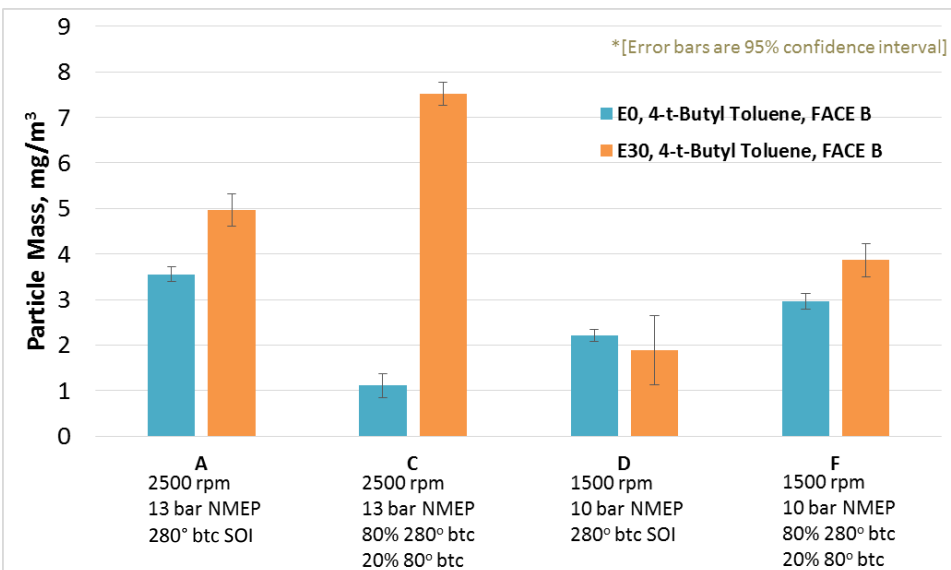






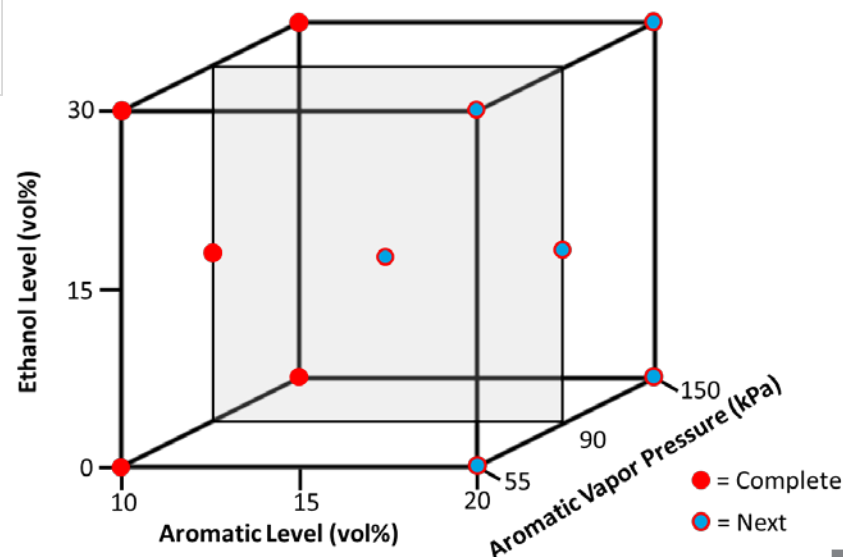
Demonstrated that under some conditions increased heat of vaporization can cause heavy aromatics to form more PM

## Approach and Technical Accomplishments/Progress



- GDI single cylinder engine
- PM mass by AVL Microsoot sensor, dilute, denuded exhaust
- Compares E0 and E30 blends at constant t-butyltoluene vol%

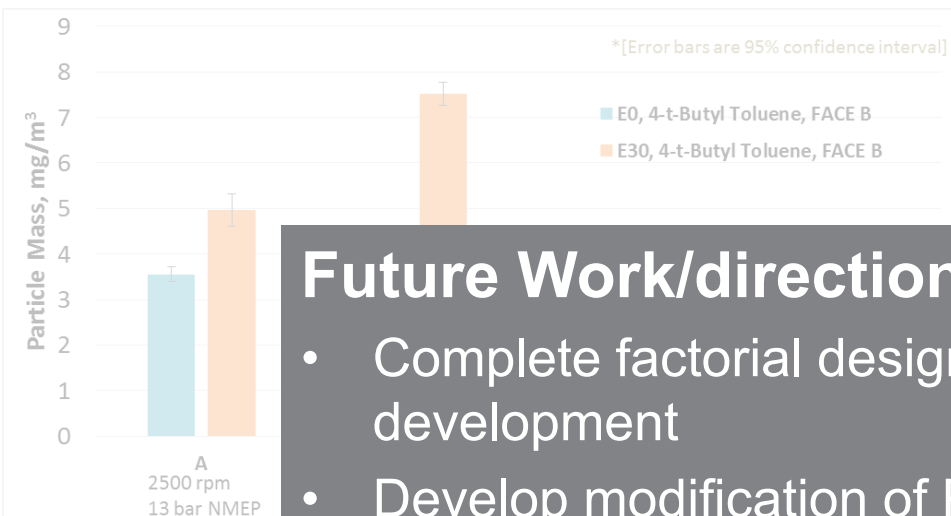
- Factorial experimental design to quantify competing effects of
  - dilution (reduces PM)
  - evaporative cooling (increases PM)
- Dilution effects dominating for more highly volatile aromatics than tert-butyltoluene at 10 vol%





Demonstrated that under some conditions increased heat of vaporization can cause heavy aromatics to form more PM

## Approach and Technical Accomplishments/Progress



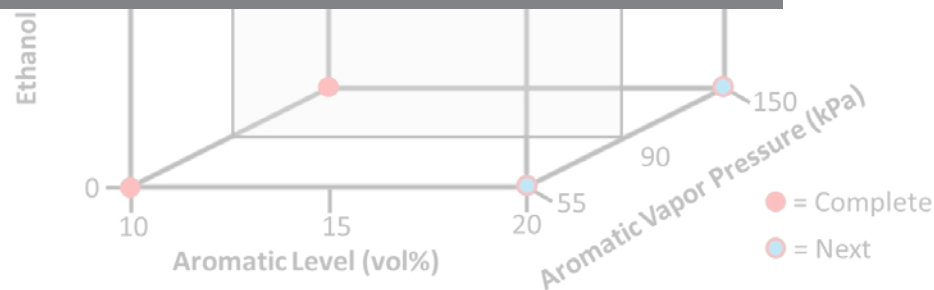
- Factorial experimental design to quantify competing effects of
  - dilution (reduces PM)
  - evaporative cooling (increases PM)

## Future Work/directions

- Complete factorial design and regression model development
- Develop modification of PMI to accommodate evaporative cooling effects and oxygenate chemistry
- Examination of injection strategies and parameters to leverage fuel properties to avoid PM emissions

*Any proposed future work is subject to change based on funding levels*

- GDI single
- PM mass sensor, exhaust
- Compares E0 and E30 blends at constant t-butyltoluene vol%



# Project Summary #4



## Oak Ridge National Laboratory

### **PM formation and oxidation fundamentals (\$376K)**

1.3.2 Fuel Impact on GDI PM Formation and Gaseous Emissions During Cold Start

1.3.3 Fuel Contribution to PM From Kinetically-Controlled Combustion

**John Storey and Melanie DeBusk (co-PIs)**





# Relevance

## **Overall Objective**

- Emission regulations dictate use of aftertreatment hardware
  - GPF may be required to meet 2025 PM Regulations (1 mg/mile)
  - GPF causes backpressure – reducing engine efficiency, increasing LSPI potential
- Study how PM is affected by advanced fuel properties and bio-blend fuels being considered to improve overall efficiency
  - Increased oxygenate content (i.e. oxygenated bio-blends)
  - Chemical properties of bio-blend (functional groups and level of saturation)
- Evaluate merit function PM control term to predict fuel sooting

## **FY17 Objective**

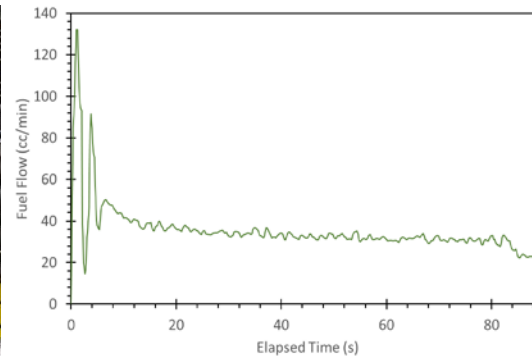
- Cold-Start major contributor to PM mass during FTP drive cycle
- Isolate initial cold-start PM production as function of fuel properties
  - How does oxygenated fuel follow PMI based PM predictions?
  - Does Cold-Start PM follow PMI index?
  - Does PMI control term in Merit Function capture this trend?
  - Statistical confidence in results



# Approach

A 2.0 L start-cart with forced cooling allowed 12-16 cold-starts per day was used to collect PM from during a Cold-Start Transient (90s). Dry-Soot and PM production sampled to study fuel sooting levels for multiple fuel blends to evaluate how different oxygenated fuel blends impact PM during high sooting engine operation.

## Cold-start fueling strategy using Start-Cart



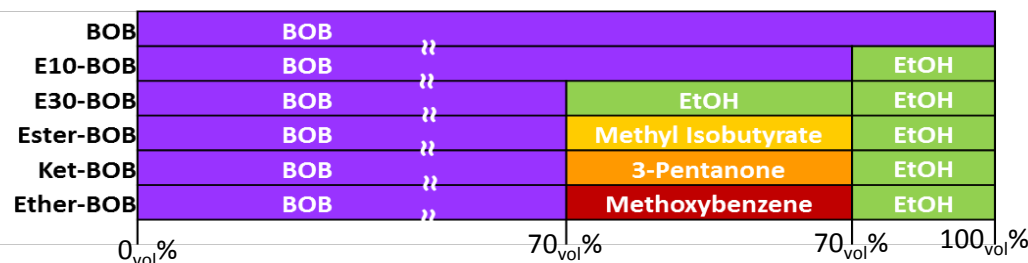
- Coolant in/out, Engine Head and Block and oil sump (16-19°C)
- CO<sub>2</sub> measurements from all fuels studied within 1% (bag sampling)

## Oxygenated Fuel Blends Studied:

Splash blending with BOB used to make Co-Optima E30

\*E0-c : Tier II E0 Lube Certification fuel

\*E10-c: Tier III E10 Certification fuel



## Statistical Confidence in Results

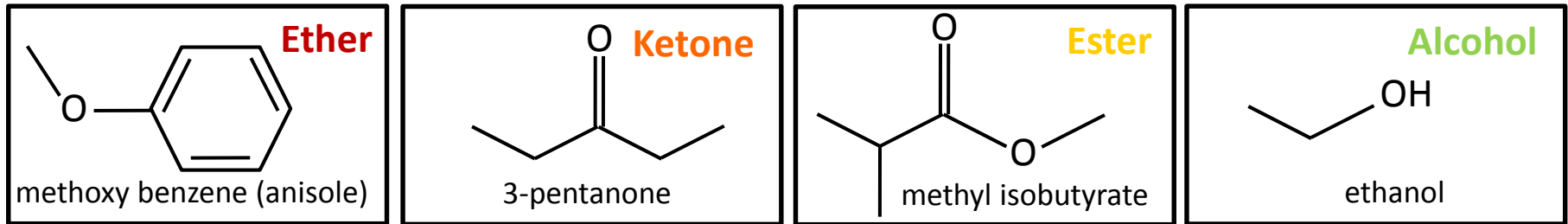
- On-line measurement
  - 18 cold-starts transients per fuel
  - AVL Micro Soot Sensor measurements
- Gravimetric Mass Sampling
  - Triplicate filter samples per fuel
  - 6 cold-starts per filter





# Approach

A 2.0 L start-cart with forced cooling allowed 12-16 cold-starts per day was used to collect PM from during a Cold-Start Transient (90s). Dry-Soot and PM production sampled to study fuel sooting levels for multiple fuel blends to evaluate how different oxygenated fuel blends impact PM during high sooting engine operation.



Does chemical functionality of oxygenated bio-fuel impact PM?

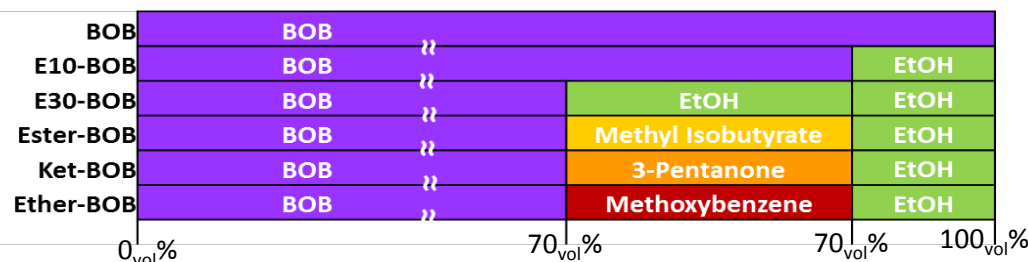
- Mass, Number, Size and/or Chemistry

## Oxygenated Fuel Blends Studied:

Splash blending with BOB used to make Co-Optima E30

\*E0-c : Tier II E0 Lube Certification fuel

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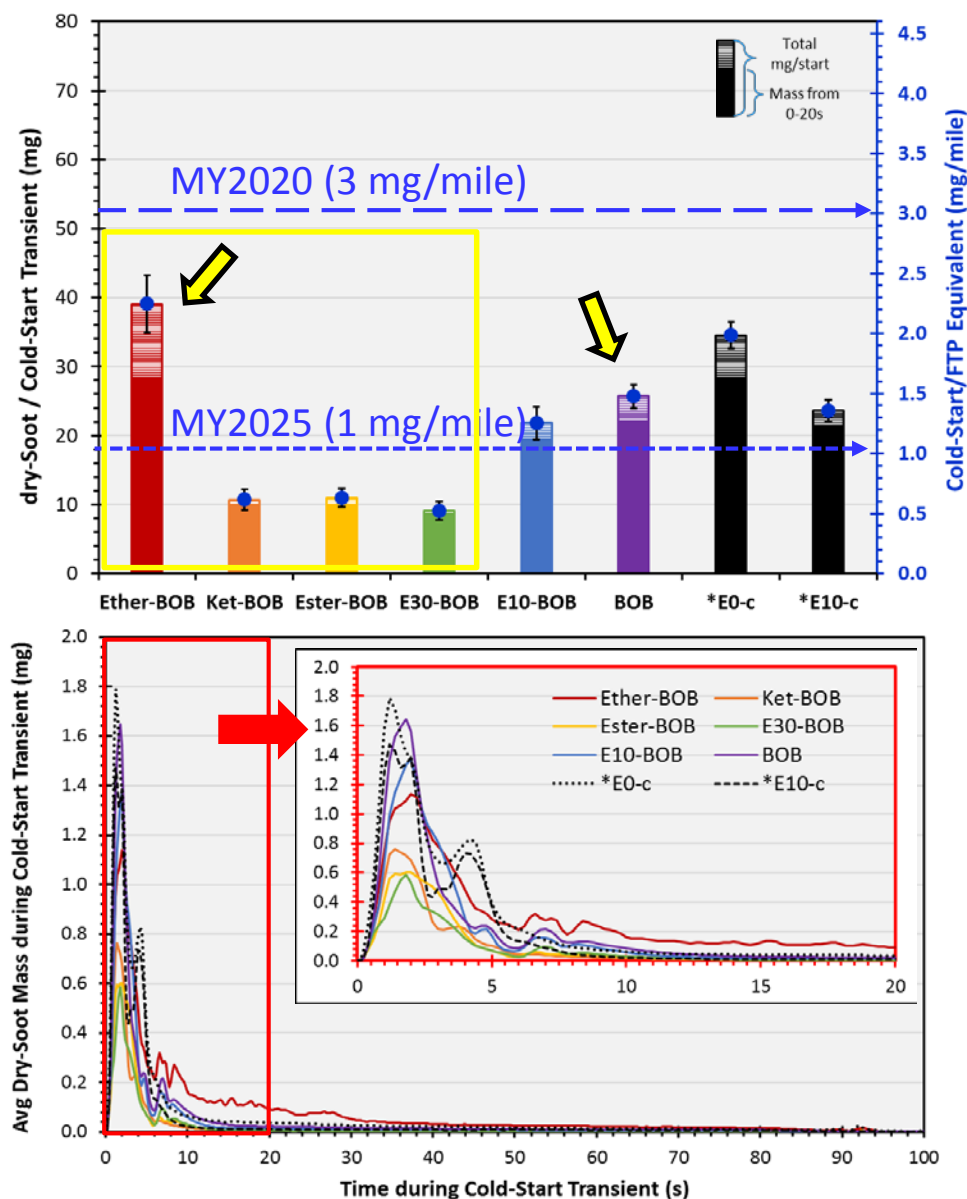


## Statistical Confidence in Results

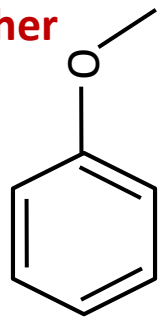
- On-line measurement
  - 18 cold-starts transients per fuel
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- Gravimetric Mass Sampling
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# Oxygenated Fuel Blends Impact on dry-Soot Mass

On-line measurement (AVL Microsoot Sensor)



- 30<sub>vol</sub>% Oxygenate Fuels
    - Typically showed a significant reduction in dry-soot
    - **Ether-BOB** (anisole)
      - More soot than **BOB**
      - ~4x the mass of other 30% oxygenated fuels
- Ether**

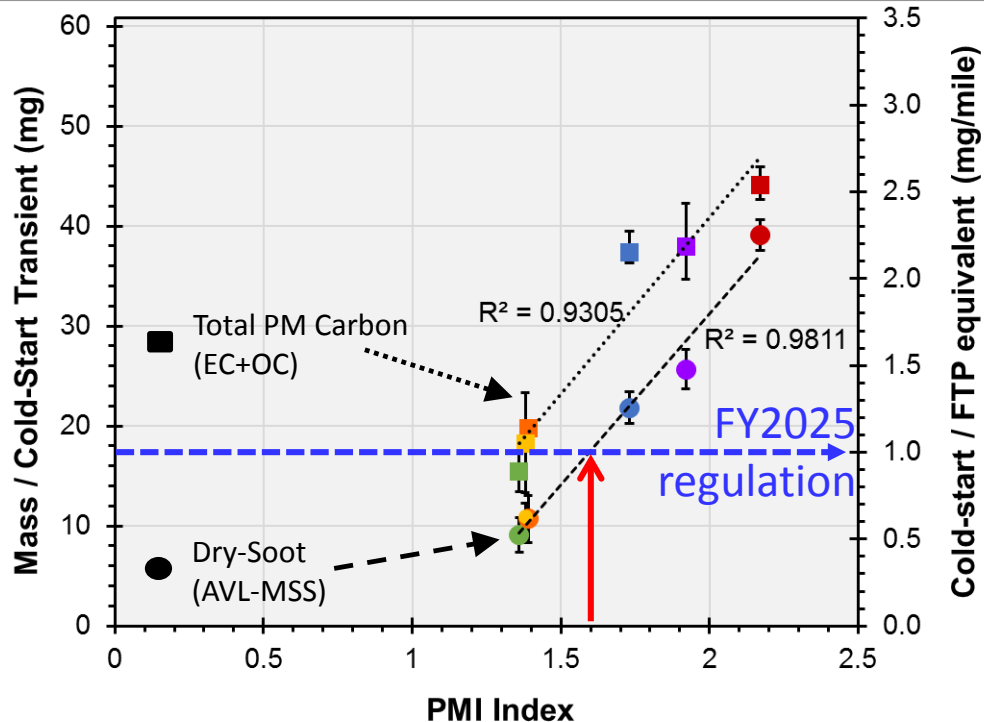


methoxy benzene

- contains 20<sub>vol</sub>% methoxybenzene an oxygenated aromatic
  - Impact of functional group or double bonds?
- First 20s of cold-start transient
    - Soot production profile varies by fuel
    - Most of soot produced (by mass)



# Cold-Start Sooting Trend Predicted by PMI



**Ether - BOB**

**Ketone - BOB**

**Ether - BOB**

**E30 - BOB**

**E10 - BOB**

**BOB**

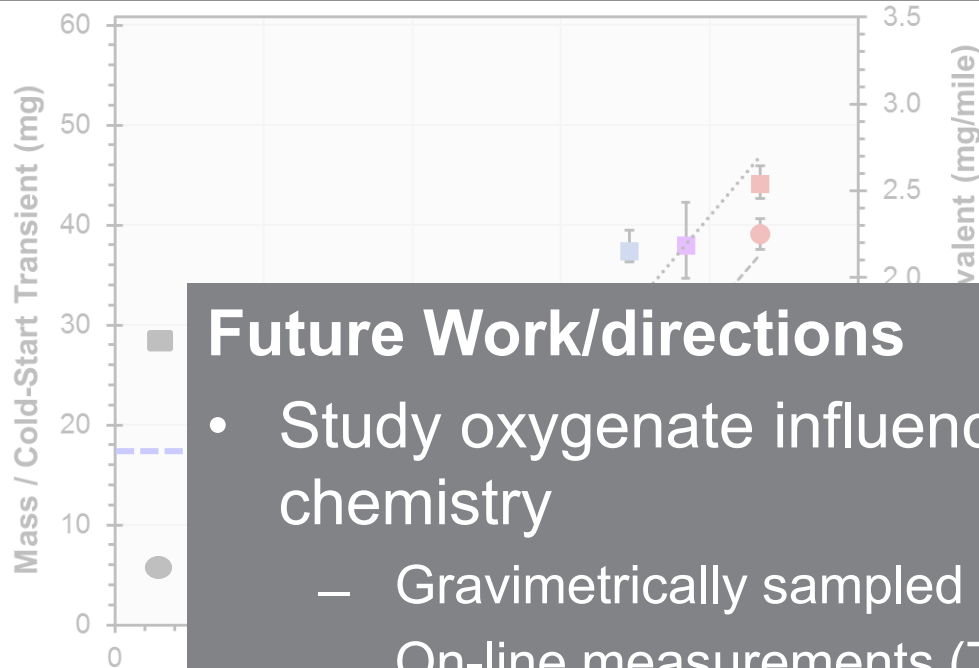
**Merit Function  
PM Control Term**

$$- H(PMI - 1.6) \times [0.7 + 0.5(PMI - 1.4)]$$

- Mass quantity of PM will dictate need for a particulate filter (PF)
- Merit Function's PM Control Term uses PMI to predict need for PF
  - In cylinder control and use of a PF can cause a decrease in efficiency
- Cold-start dry-soot data supports update of -H(X) function
  - From 2.0 to 1.6
- Total PM carbon (EC + OC) shows greater PM mass but trend follows PMI



# Cold-Start Sooting Trend Predicted by PMI



## Future Work/directions

- Study oxygenate influence on GDI cold-start PM chemistry
  - Gravimetrically sampled PM
  - On-line measurements (TSI-EEPS)
- Study potential pathways to ACI PM organic carbon and its formation
  - Organic carbon is the main constituent in ACI exhaust PM
- Cold-start dry-soot data supports update of -H(X) function
  - From 2.0 to 1.6
- Total PM carbon (EC + OC) shows greater PM mass but trend follows PMI

# Project Summary #5

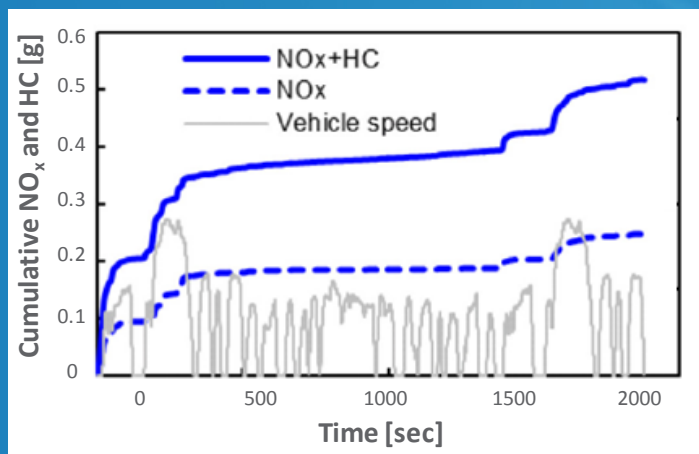


## Oak Ridge National Laboratory

### Fuel Impacts on Emissions Control Performance & Durability (\$175K)

**Todd Toops and Josh Pihl (co-PIs)**

William Brookshear and Sreshtha Majumdar

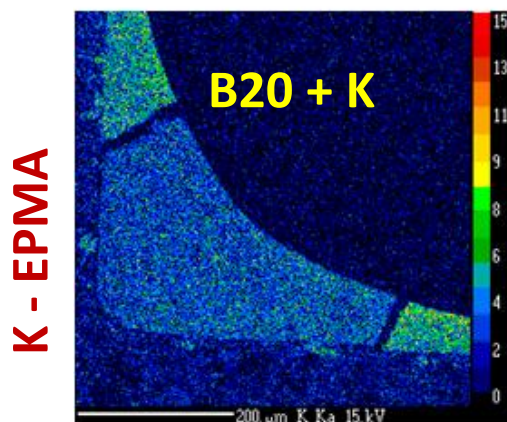




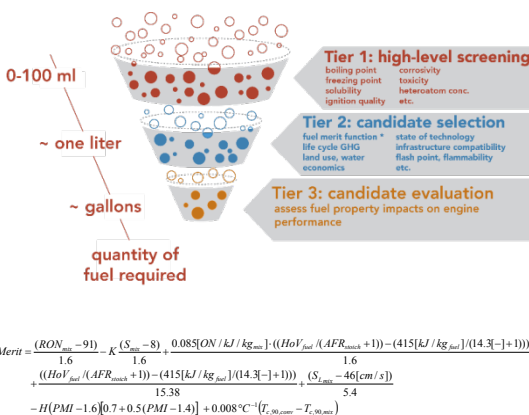


- Objective: Understand the effects of Co-Optima blendstock candidates on emissions control devices

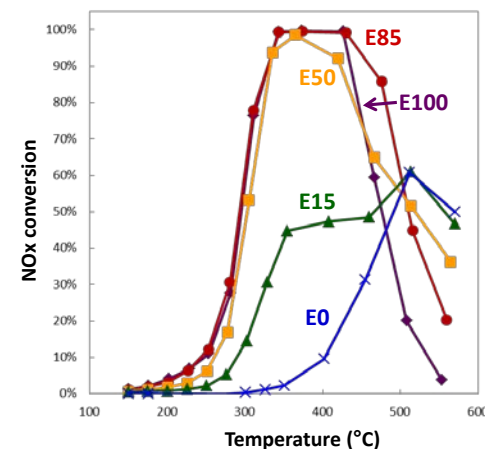
Evaluate effects of trace impurities in Co-Optima blendstock candidates



Develop screening criteria and merit function terms related to gaseous emissions



Identify opportunities to reduce emissions and fuel penalty through co-optimization



Outcome: Identification of criteria pollutant emissions control challenges and opportunities created by Co-Optima blendstock candidates



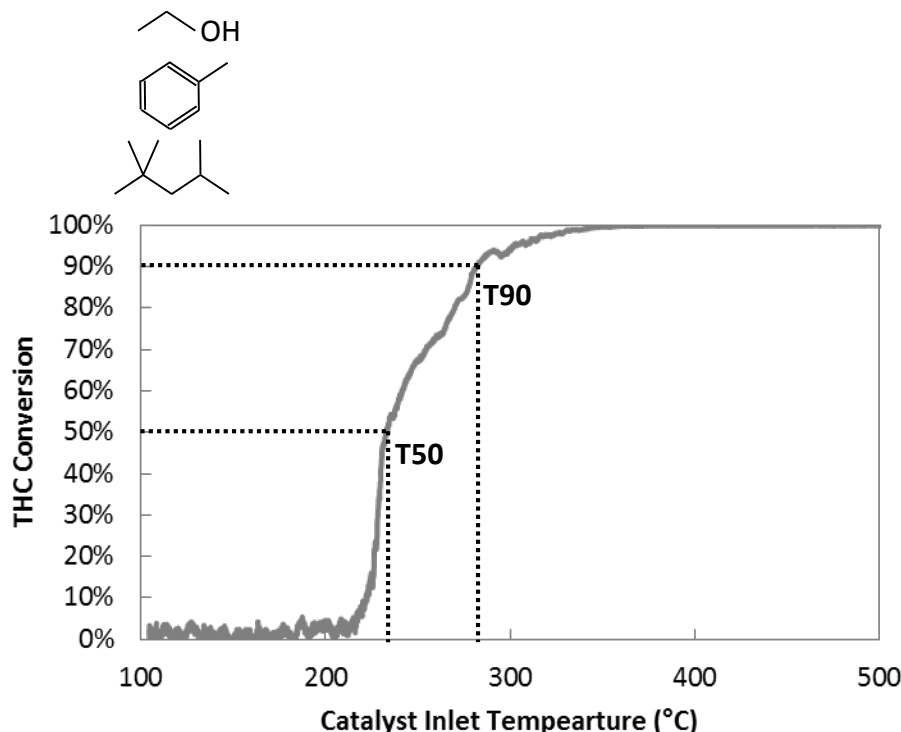
# Measuring TWC light-off temperatures of blendstocks for evaluation of Merit Function emissions control term

## Technical Accomplishments

- Developed Merit Function Emissions Control term based on cold start fuel penalty (see backup slides for details)

$$0.008\text{ }^{\circ}\text{C}^{-1}(T_{c,90,conv} - T_{c,90,CB})$$

- Measuring catalytic light-off temperatures ( $T_{c,90}$ ) of Co-Optima SI-intended blendstocks
  - aged commercial TWC
  - synthetic exhaust flow reactor
  - blendstocks**  $T_{90} \leq E10\ T_{90}$





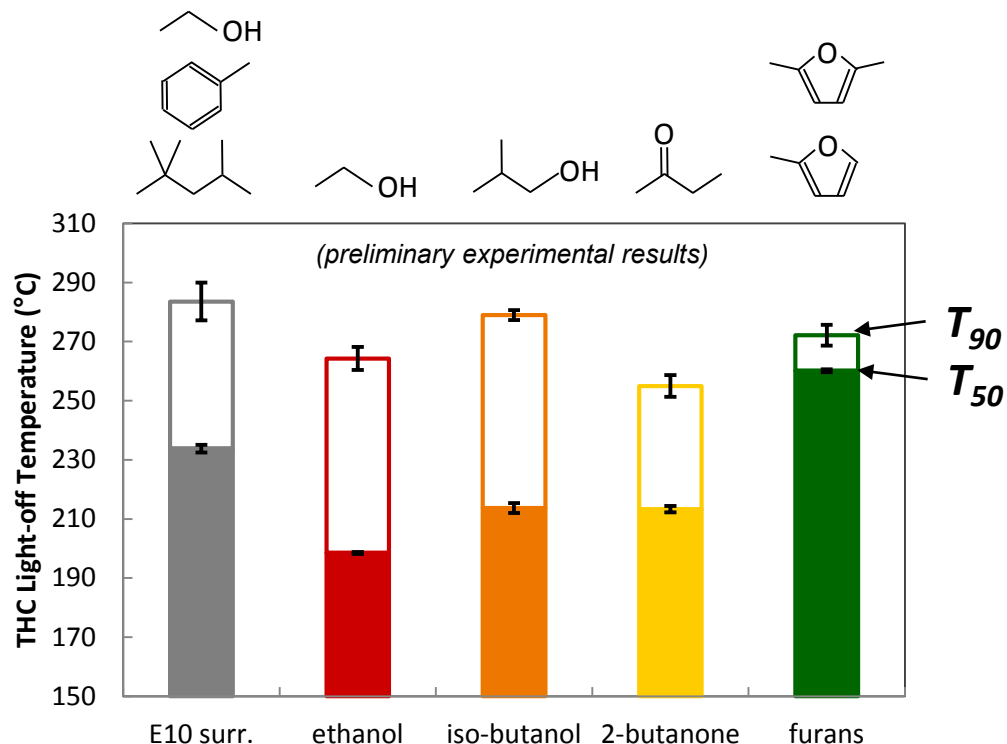
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## Technical Accomplishments

- Developed Merit Function Emissions Control term based on cold start fuel penalty (see backup slides for details)

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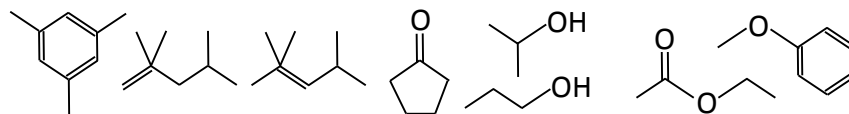
- Measuring catalytic light-off temperatures ( $T_{c,90}$ ) of Co-Optima SI-intended blendstocks
  - aged commercial TWC
  - synthetic exhaust flow reactor
  - blendstocks**  $T_{90} \leq E10\ T_{90}$



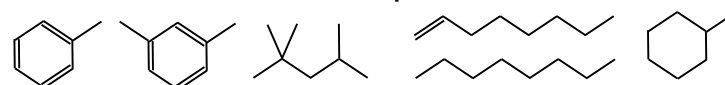
## Future Work

- FY18 plans: measure light-off temperatures for selected blends
  - develop correlation to predict blend light-off based on pure components

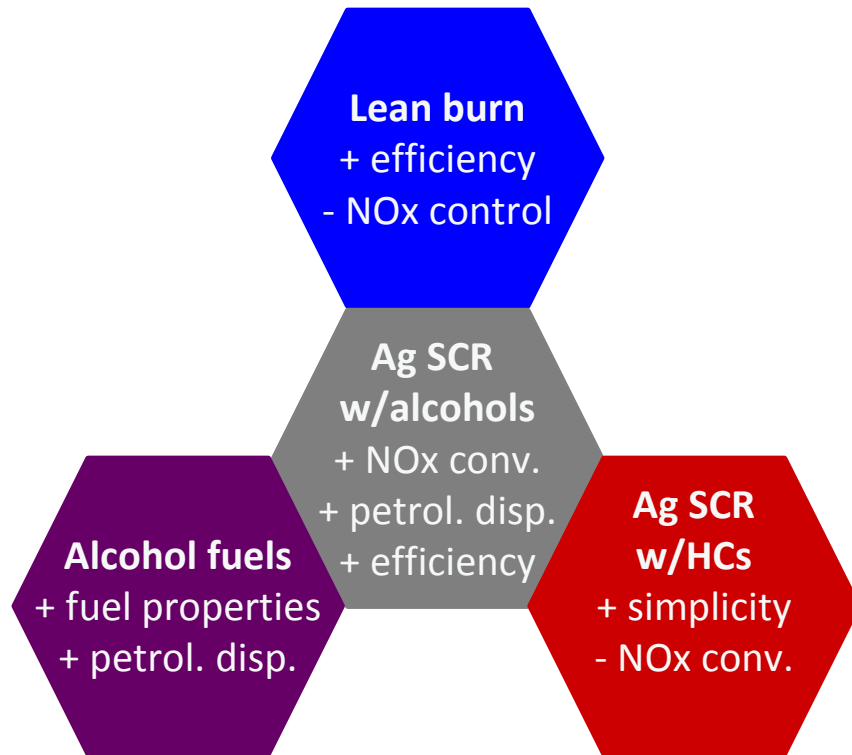
Co-Optima candidates for potential evaluation:



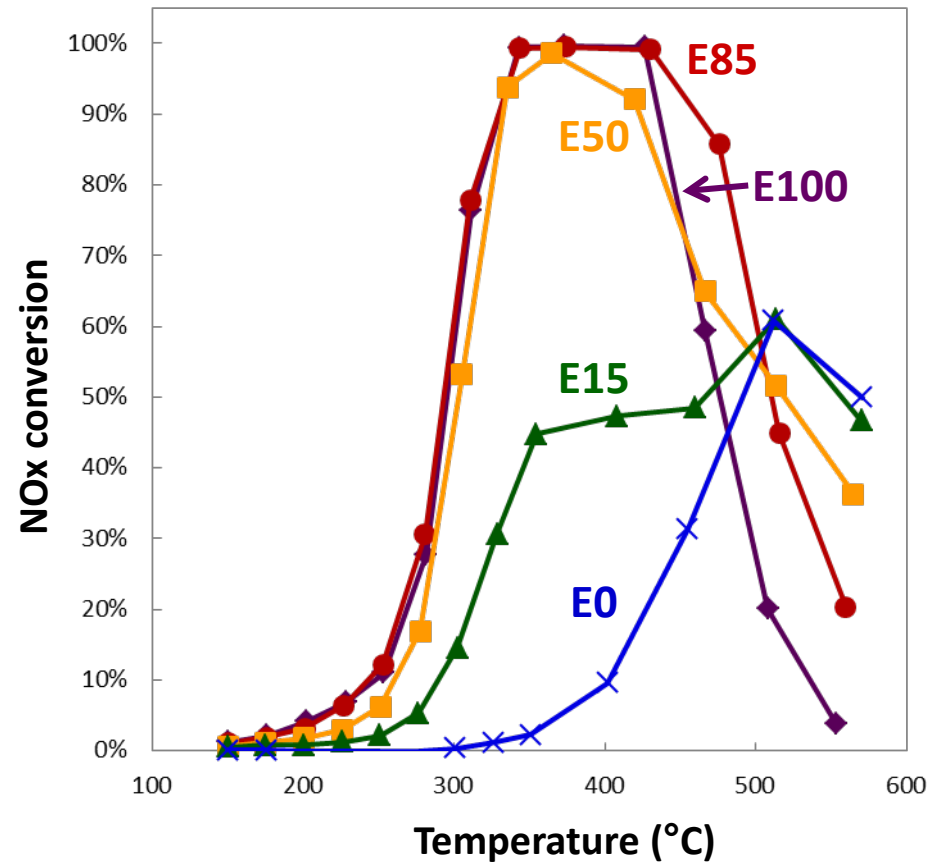
Conventional HC fuel for potential evaluation:



# NO SCR by alcohol-containing fuels could be a pathway to NO<sub>x</sub> control for SI/ACI lean burn engines



NO<sub>x</sub> conversion by ethanol/gasoline blends over a Ag catalyst



# Dual SCR approach improves emissions control performance over a Ag-only system with E85 reductant



—  —  (Ag only, steady fuel)

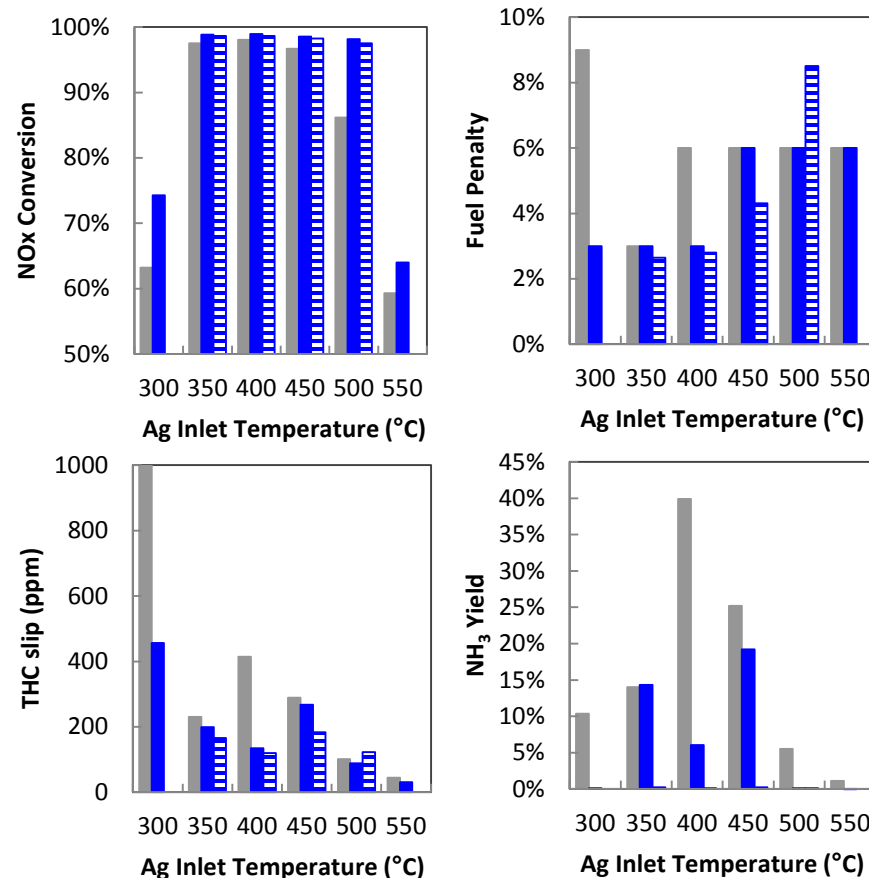
- achieves high NO<sub>x</sub> conversion efficiencies over a limited T window
- results in higher than acceptable fuel penalty, NH<sub>3</sub> yield, HC slip

—  —  —  (Ag+Cu, steady fuel)

- improves NO<sub>x</sub> conversion efficiencies
- reduces fuel penalty, NH<sub>3</sub> slip, HC slip

- - -  —  —  (Ag+Cu, fuel pulses)

- maintains high NO<sub>x</sub> conversion efficiencies
- reduces fuel penalty and HC slip
- eliminates NH<sub>3</sub> slip



Experiments conducted with Ag/Al<sub>2</sub>O<sub>3</sub> and Cu-SSZ-13 catalysts on a synthetic exhaust gas flow reactor using 15% ethanol + 85% cert. gasoline

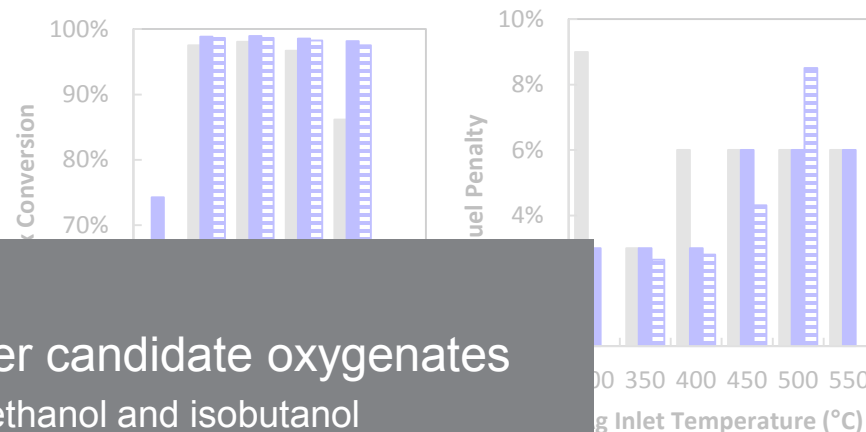




# Dual SCR approach improves emissions control performance over a Ag-only system with E85 reductant

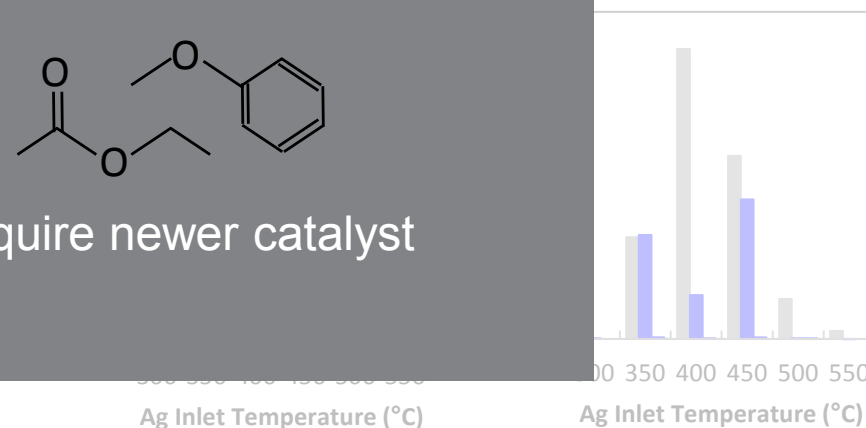
— Ag (Ag only, steady fuel)

- achieves high NO<sub>x</sub> conversion efficiencies over a limited T window
- results in fuel penalty, NO<sub>x</sub> slip



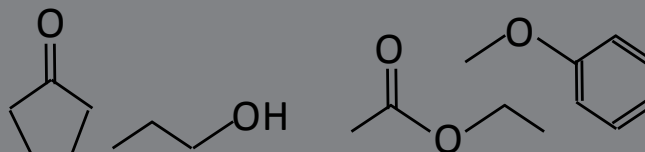
— Ag

- improves NO<sub>x</sub> conversion
- reduces fuel penalty



## Future Work/directions

- Evaluate reactivity of other candidate oxygenates
  - Have already evaluated ethanol and isobutanol



- Efforts are ongoing to acquire newer catalyst technology from Umicore

--- Ag

- maintains high NO<sub>x</sub> conversion efficiencies
- reduces fuel penalty and HC slip
- eliminates NH<sub>3</sub> slip

Experiments conducted with Ag/Al<sub>2</sub>O<sub>3</sub> and Cu-SSZ-13 catalysts on a synthetic exhaust gas flow reactor using 15% ethanol + 85% cert. gasoline



- **Co-Optimization of Fuels and Engines** brings together expertise from across the National Laboratory system, working toward a common purpose. This effort has stakeholder engagement at a high level to ensure relevance.
  - 9 laboratories, engines, fuels, kinetics, simulation, biofuel development, LCA& TEA, market transformation
  - Monthly stakeholder engagement phone calls, industry listening days, external advisory board
- Projects presented at the semi-annual AEC program review meetings
- Engagement with ACEC Tech Team activities

## **Additional project-level collaborations with industry and academia:**

- **NREL: Particulate Matter Index (PMI) refinement**
  - Colorado State University
- **ORNL: Fuel Impacts on Emissions Control Performance & Durability**
  - University of Michigan - Galen Fisher
  - Emissions Solutions (currently CDTi – Clean Diesel Technologies, Inc.)

# Response to last year's AMR scores



- **Approach:** *getting an early look at the engine out emissions would help downselect candidate fuels and regimes*...spray work feeding into the modeling team is a critical effort that should be continued...emissions work looking at fuel impurities is critical to get an early look at impact of biofuels
- **Technical Accomplishments:** technical accomplishments to date are impressive ... projects on the spray and emission control research were much better ... *it is not clear how the planned emissions activities will address emissions control for LTC or ACI engine concepts*
- **Collaborations:** collaborative work between the labs is impressive ... *collaborations with external stakeholders and companies is either not presented or at a low level*
- **Future plans:** spray and emissions research outlined for future work is very relevant ... *proposed projects and work is scattered with no clear plan to determine winners and losers*
- **Relevance:** the emissions research is expected to contribute to achieving improved engine efficiency along with lower emissions ... *it is not clear that the Thrust II technologies will prove to be more fuel efficient and displace petroleum*
- **Resources:** *the project needs resources to look at toxics and other unintended consequences* ... *Thrust II does not have a clear focus and seems a bit excessive, especially given that this technology is more than 15 years away and not the current focus of OEMs*

## Responsive Actions

- |   |
|---|
| 1. <i>When Thrust II/ACI engine research ramps up emissions measurements will absolutely be a significant part of the effort</i>  |
| 1. <i>Lean gasoline approach currently being investigated is focused on a Thrust I/Thrust II (SI/ACI) multimode operation; more thrust II ramping up next FY; researchers have low temperature catalyst projects to draw from</i> |
| 1. <i>Engagement is primarily through the advisory board and stakeholders group of Co-optima</i>  |
| 1. <i>Co-optima not organized to pick winners and loser, but to provide relevant data for industry to make decisions in a coordinated fashion</i>   |
| 1. <i>Lean operation generally has the potential to be more efficient, but fully understanding all sides of the efficiency questions is a goal of program</i>   |
| 1. <i>Additional funding always appreciated, but funding levels expected to be flat</i><br>2. <i>Important considerations being discussed at the leadership level</i>   |



## Relevance

- Understanding fuel effects on spray structure and on aftertreatment devices is central to the co-optimization of fuels and engines
- Determining fuel impact on PM is critical for predicting or avoiding PF for 2025 PM Regulations
- Understanding fuel impact on emissions and emissions control critical for meeting regulations, avoiding deactivating impurities and understanding potential opportunistic chemical behavior

## Approach

- Individual projects are coordinated to a high degree and seek to build on the strengths of the labs

## Accomplishments

- Establishing spray capabilities for flammable co-optima fuels at two national laboratories
- Evaluation of PMI for oxygenated fuels through factorial design and cold-start evaluation
- Assessing impact of fuels TWC light off behavior of pure compounds under consideration for SI
- Highlighting synergistic behavior of ethanol and silver and copper catalysts for dual SCR of NOx

## Collaborations

- “Co-Optima” has 9 National Labs, stakeholder engagement, and external advisory board
- Projects presented at AEC semi-annual program review, engaged with ACEC TT, SAE World Congress and Co-Optima All-Hands Meeting

## Future Work

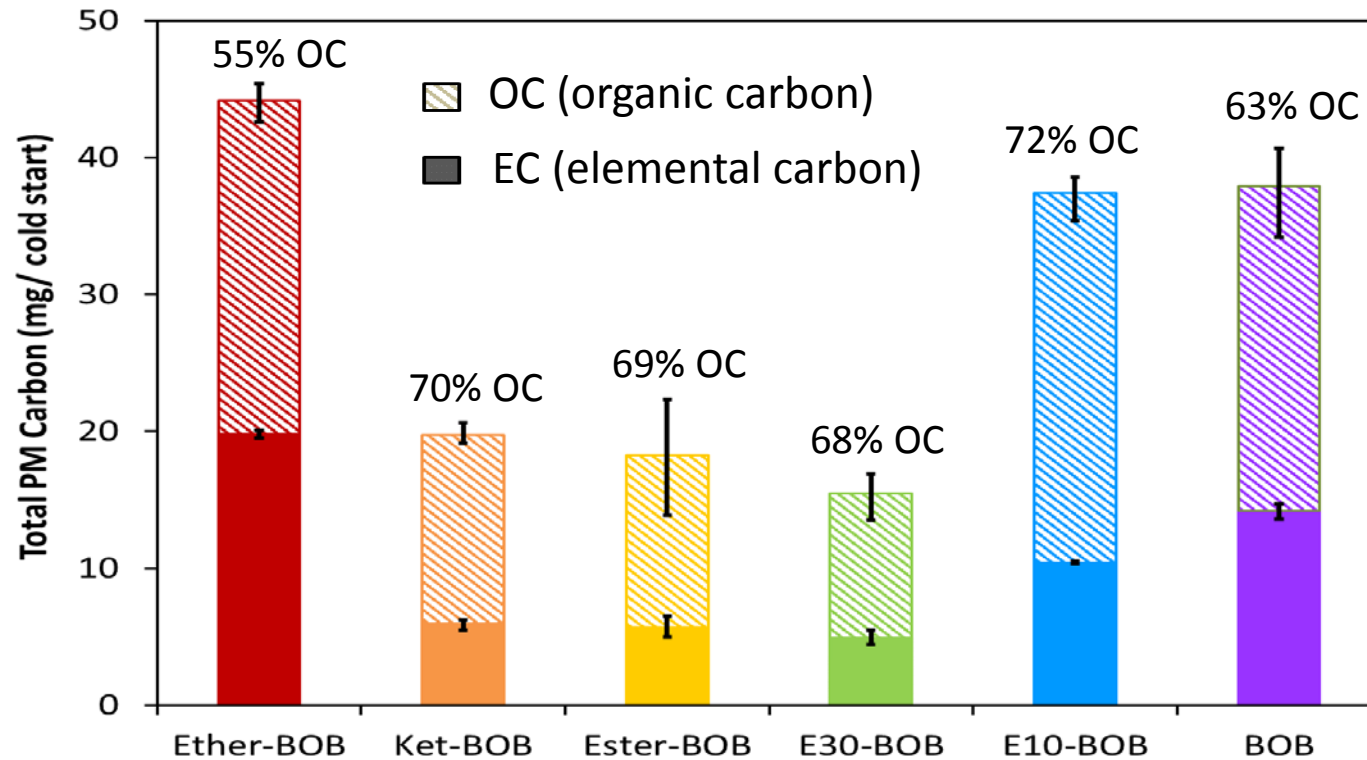
- Spray research will start evaluating Co-Optima fuels very soon
- PMI factorial experimentation will be completed and adjustments to the PMI term will be evaluated
- Complete analysis of cold-start collected PM and identify pathway to PM formation based on fuel
- Complete TWC light-off evaluation of Co-optima SI-fuels and evaluate other oxygenates in dual SCR technique

*Any proposed future work is subject to change based on funding levels*



## TECHNICAL BACK-UP SLIDES

# Organic Carbon dominates Cold-Start PM

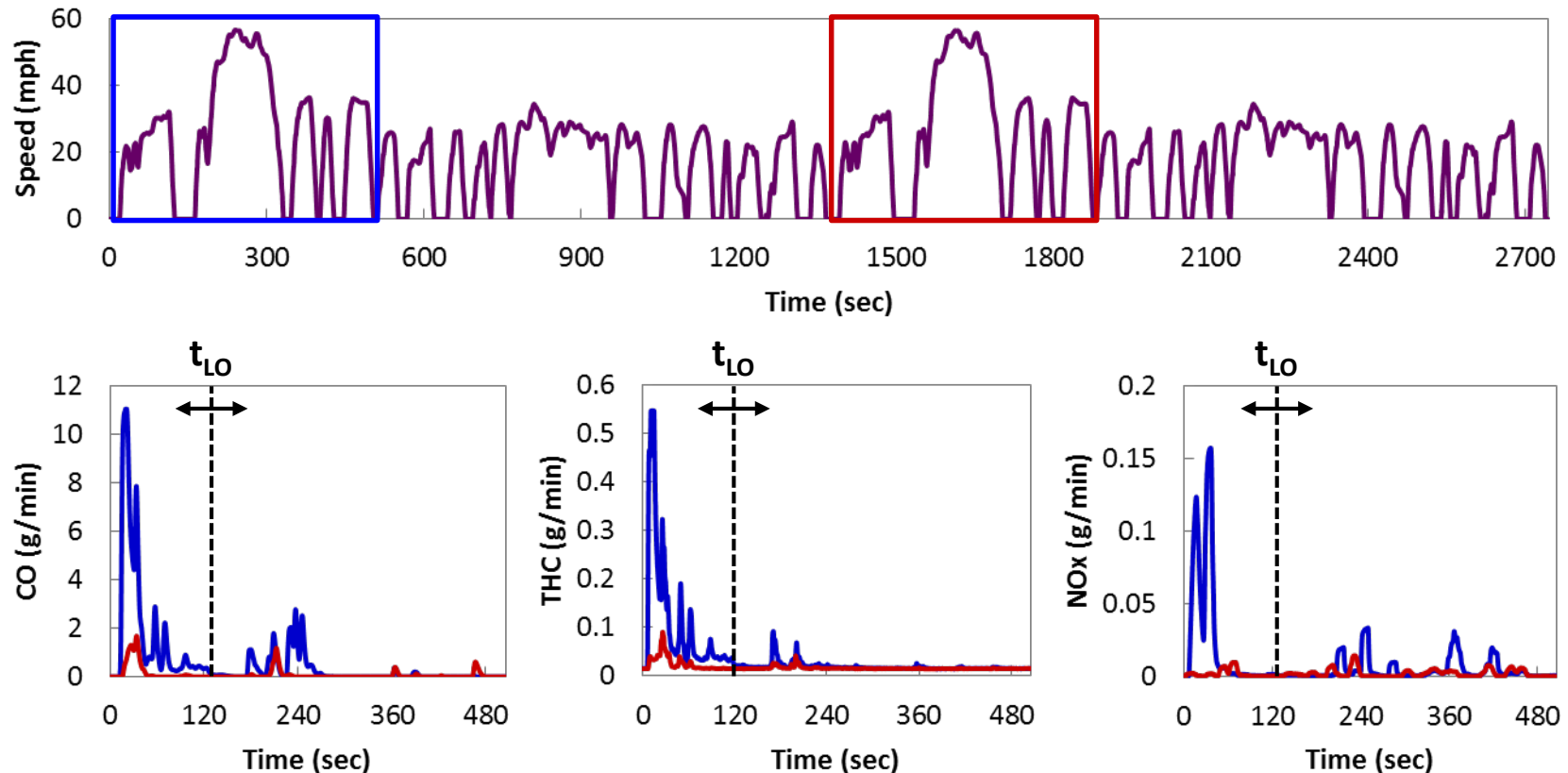


- Gravimetric quartz filter sampling
  - NIOSH 450 method for ec/oc analysis
  - Triplicate filters (6 cold-starts per filter)
- Greater than 50% of PM is considered OC for all fuels



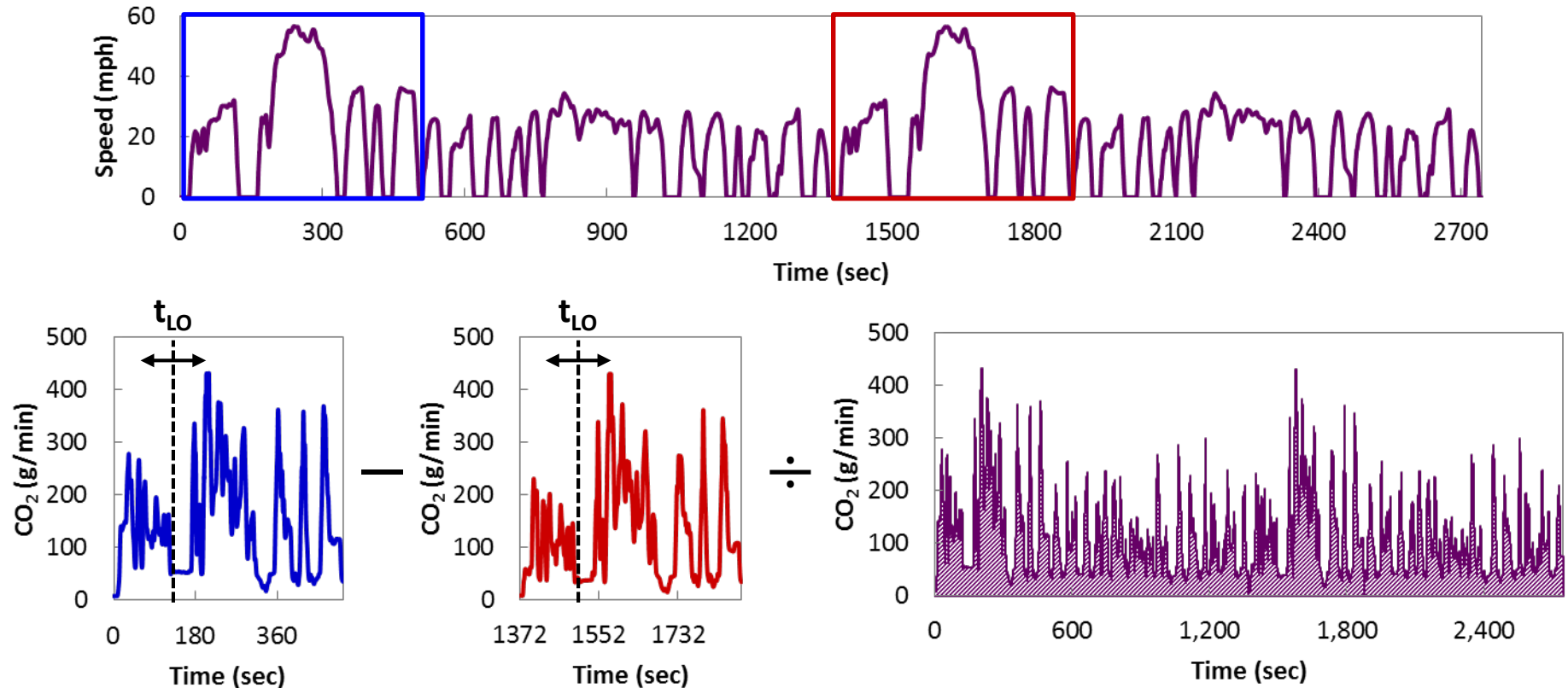


# Development of a SI Merit Function Emissions Control Term Based on FTP Cold Start Fuel Penalty



- Need method to correlate emissions performance with fuel efficiency for inclusion in SI merit function
- Most emissions for stoichiometric SI engines released during cold start
- Extra fuel burned during cold start to heat catalyst decreases efficiency

# Development of a SI Merit Function Emissions Control Term Based on FTP Cold Start Fuel Penalty



- Cold start fuel penalty = (hot start CO<sub>2</sub> - cold start CO<sub>2</sub>) ÷ total FTP CO<sub>2</sub>
- Cold start fuel penalty proportional to catalyst light-off time, which depends on light-off temperature, which will vary with fuel composition

$$\frac{\Delta F_{LO,conv} - \Delta F_{LO,CB}}{F_{FTP}} \approx \frac{\Delta f_{LO}}{F_{FTP}} (t_{LO,conv} - t_{LO,CB}) \approx \frac{\Delta f_{LO}}{F_{FTP}} \alpha (T_{c,90,conv} - T_{c,90,CB}) \approx 0.008 \text{ } ^\circ\text{C}^{-1} (T_{c,90,conv} - T_{c,90,CB})$$

# Cold-Start FTP Equivalent Calculation



$$\left[ \frac{m' + m''}{D' + D''} * 0.43 \right] + \left[ \frac{m''' + m''}{D' + D''} * 0.57 \right] = Y$$

$$\left[ \frac{m' + m''}{D' + D''} * 0.43 \right] = \left[ \frac{X'}{7.47} * 0.43 \right] + \left[ \frac{X}{7.47} * 0.43 \right]$$

$$X' + X = m'$$

$$D' + D'' = 7.47 \text{ miles}$$

Therefore,  $\frac{X'(mg)}{7.47 \text{ (miles)}} * 0.43 = Y' (mg/mile)$

$X'$  = PM per (90s) cold-start transient (mg)

$Y'$  = Cold-start PM FTP equivalent (mg/mile)

$Y$  = Total FTP PM rate (mg/mile)

$X$  = mass of PM from FTP Bag 1 after 90s transient

$m'$  = mass of PM from FTP Bag 1

$m''$  = mass of PM from FTP Bag 2 and 4

$m'''$  = mass of PM from FTP Bag 3

$D'$  = FTP miles for Bag 1 and 3

$D''$  = FTP miles for Bag 2 and 4

